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Multiscale Thermohydrologic Model Analysis of Heterogeneity and Thermal-Loading Factors for the Proposed Repository at Yucca Mountain

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INTRODUCTION

The MultiScale ThermoHydrologic Model (MSTHM) predicts thermohydrologic (TH) conditions in emplacement drifts and the adjoining host rock throughout the proposed nuclear-waste repository at Yucca Mountain. The MSTHM is a computationally efficient approach that accounts for TH processes occurring at a scale of a few tens of centimeters around individual waste packages and emplacement drifts, and for heat flow at the multi-kilometer scale at Yucca Mountain. We present recent MSTHM simulations that address the influence of repository-scale thermal-conductivity heterogeneity and the influence of preclosure operational factors affecting thermal-loading conditions. We can now accommodate a complex repository layout with emplacement drifts lying in non-parallel planes using a superposition process that combines results from multiple mountain-scale submodels. This development, along with other improvements to the MSTHM, enables more rigorous analyses of preclosure operational factors. These improvements include the ability to (1) predict TH conditions on a drift-by-drift basis, (2) represent sequential emplacement of waste packages along the drifts, and (3) incorporate distance- and time-dependent heat-removal efficiency associated with drift ventilation. Alternative approaches to addressing repository-scale thermal-conductivity heterogeneity are investigated. We find that only one of the four MSTHM submodel types needs to incorporate thermal-conductivity heterogeneity. For a particular repository design, we find that the most influential parameters are (1) percolation-flux distribution, (2) thermal-conductivity heterogeneity within the host-rock units, (3) the sequencing of waste-package emplacement, and (4) the duration of the preclosure ventilation period.

WORK DESCRIPTION

The MSTHM calculates the following TH variables: temperature, relative humidity, liquid-phase saturation, liquid-phase flux, gas-phase composition, gas-phase pressure, capillary pressure, water-vapor flux, air flux, and evaporation rate. MSTHM variables are determined at various generic locations in the emplacement drifts and in the near-field host rock surrounding the drifts. The MSTHM has been used extensively in the Yucca Mountain Project [1,2,3,4]. It is also described in Buscheck et al. [5] and CRWMS [6]. The MSTHM consists of four submodel types, all of which are run using the NUFT computer code [7]. These four submodels are the following:

- SMT (3-D Smeared-heat-source, Mountain-scale, Thermal-conduction)
- LDTH (2-D Line-averaged-heat-source, Drift-scale, ThermoHydrologic)
- SDT (1-D Smeared-heat-source, Drift-scale Thermal-conduction)
- DDT (3-D Discrete-heat-source, Drift-scale Thermal-conduction-radiation)

For the MSTHM calculations, LDTH and SDT submodels are run at many geographic locations that are distributed uniformly over the repository area; these submodels use the stratigraphy, overburden thickness, TH boundary conditions, and percolation fluxes appropriate for each location. At each geographic location, the LDTH- and SDT-submodel calculations are conducted at different values of thermal loading, which can be quantified by Areal Mass Loading (AML), expressed in terms of metric tons of uranium per acre (MTU/acre). The *modeled* AML is obtained by virtue of the selected drift spacing in the LDTH- or SDT- submodel. The *emplaced* AML for the repository is obtained by averaging the total repository inventory of 70,000 MTU over the entire heated repository footprint. The 70,000 MTU includes 63,000 MTU of commercial spent-nuclear-fuel (CSNF) waste packages and 7000 MTU of high-level-waste (HLW) waste packages [8]. The results from submodels with modeled AMLs less than the emplaced AML account for the evolving influence of the edge-cooling effect (i.e., waste-package locations close to the repository edges cool faster than those at the center). The results from submodels with modeled AMLs higher than the emplaced AML account for waste packages with greater-than-average heat output.

The LDTH submodel domain is a 2-D drift-scale cross-section, perpendicular to the drift axis, extending from the ground surface down to the water table. The LDTH submodels include coupled TH processes and assume a heat-generation history that is effectively that of the entire waste-package inventory line-averaged over the total heated length of emplacement drifts in the repository. Three-dimensional SMT submodel results are combined with LDTH-submodel results through an interpolation process using a parameter termed the 'host-rock-effective AML'. Combining the SMT-submodel results with the LDTH-submodel results accounts for the influence of mountain-scale heat flow (including the edge-cooling effect) on local TH behavior. At this stage, the MSTHM is equivalent to a Line-averaged-heat-source, Mountain-Scale Thermo-Hydrologic (LMTH) model.

The influence of waste-package-to-waste-package deviations in local temperatures is addressed with the DDT submodels. The DDT submodels, which include ten discrete waste packages, are run at the modeled AMLs. The DDT submodels represent thermal conduction in the emplacement drifts and host rock, as well as thermal radiation between the surfaces of the open cavities in the emplacement drifts. The influence of natural convection within the drifts is approximated using an effective thermal conductivity. Adding the waste-package-dependent temperature deviations calculated by DDT submodels onto the LMTH-model predictions then results in the final MSTHM output, which is equivalent to a Discrete-heat-source, Mountain-scale, ThermoHydrologic (DMTH) model.

Recent improvements to the MSTHM include the ability to (1) represent a more complicated repository layout, (2) account for repository-scale thermal-conductivity K_{th} heterogeneity in the host-rock, and (3) address detailed preclosure operational factors. Representing a more complicated repository layout is accomplished through the superposition of multiple SMT submodels. Repository-scale host-rock K_{th} heterogeneity is assembled from a series of realizations generated by James Ramsey at Sandia National Laboratory [9]. Analyses of preclosure operational factors is facilitated by recently-developed capability to (1) predict TH conditions on a drift-by-drift basis for each 20-m interval along every emplacement drift, (2) represent sequential emplacement of waste packages along the drifts, (3) incorporate distance- and time-dependent heat-removal efficiency associated with drift ventilation, and (4) represent the influence of repository-scale K_{th} heterogeneity within the host-rock units.

In a recent MSTHM analysis of a long-duration preclosure ventilation case, a repository layout with multiple non-parallel emplacement planes (Figure 1) is accommodated using a superposition process that combines results from two SMT submodels (Figure 2). This is justified by the linearity of the transient thermal conduction equation, which can accommodate K_{th} heterogeneity between and within the respective hydrostratigraphic units. The superposition process has been validated for several heterogeneous K_{th} realizations.

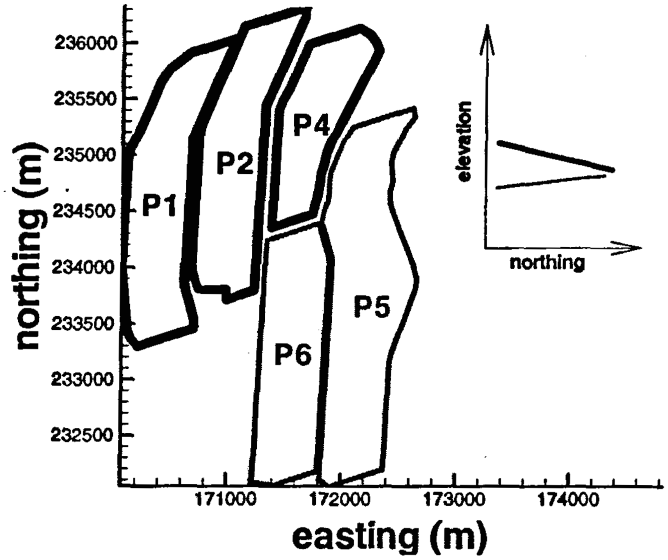

Figure 1. The repository layout considered in a recent MSTHM study. This layout includes multiple non-parallel emplacement planes. Panels P1, P2, and P4 lie in one plane (depicted with the inset's heavy sloping line). Panels P5 and P6 lie in a second plane (depicted by the inset's lighter sloping line). Panel P3 (not shown) is a "contingency" panel that is not emplaced with waste packages for the scenarios analyzed in this study.

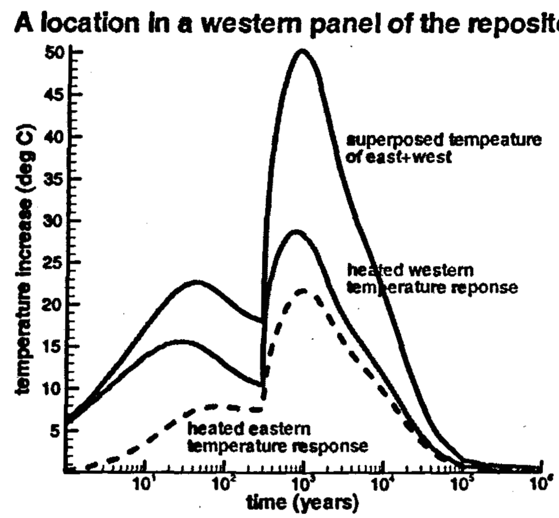

Figure 2. The superposition process combines the results from multiple SMT submodels. Computational demands of representing the complex 3-D details of the layout of the emplacement drifts and multiple panels can be distributed to multiple SMT submodels.

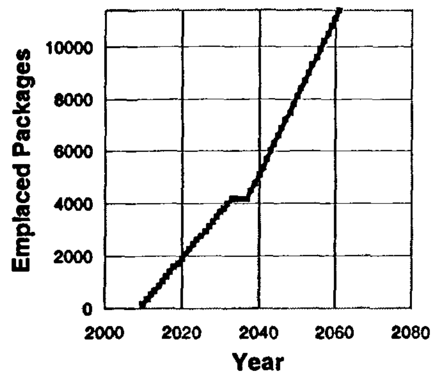

Figure 3. The simulations in this study address a repository in which waste packages are emplaced sequentially over a 52-yr period.

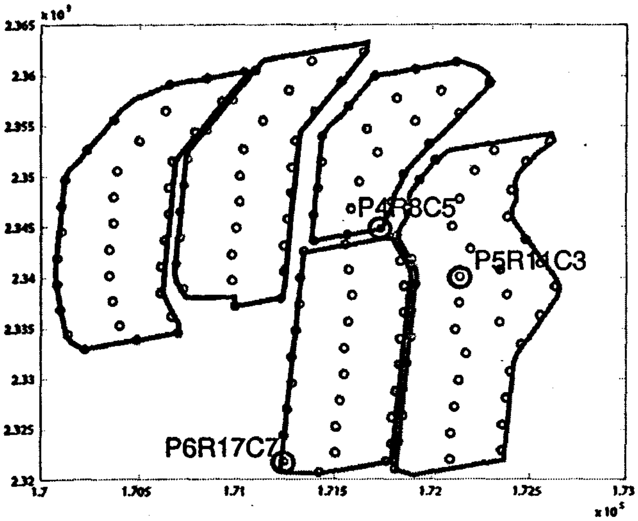

Figure 4. A total of 156 LDTH/SDT-submodel locations are available for a full macro-abstraction analysis. For this paper, the circled locations are discussed (P4R8C5, an early-loaded location; P5R11C3, a late-loaded center location; and P6R17C7, a late-loaded edge location).

Each 20-m interval of every emplacement drift is discretely represented in the SMT submodel and in the MSTHM output. Such detail allows for the accounting of the influence of sequential waste-package emplacement and distance- and time-dependent drift-ventilation heat-removal efficiency for all emplacement drifts throughout the repository. For the analysis of a long-duration preclosure ventilation case, the local start of heating and effective waste-age correspond exactly to waste-package-emplacement sequencing, a process occurring over a 52-yr period (Figure 3). The heat-removal efficiency of drift ventilation is treated as a function of time (relative to the start of ventilation) and distance (from the ventilation inlet of the emplacement drift). Note that heat-removal efficiency, which is defined to be the percentage of the waste-package heat-output removed by the ventilation air, decreases with increasing distance from the inlet of an emplacement drift. Thus, the net effective heat output from waste packages furthest removed from the inlet (i.e., immediately adjacent to the ventilation exhaust port) is greatest, while the net effective heat output from waste packages adjacent to the ventilation inlet is least. To accommodate the necessary operational details of the five-panel repository, 156 LDTH/SDT-submodel locations are required for a full macro-abstraction MSTHM analysis (Figure 4). This number of locations adequately captures the variability of infiltration flux and stratigraphy over the five-panel repository. In this study, several representative locations were selected for micro-abstraction MSTHM analyses, three of which were chosen for discussion in this paper (circled locations in Figure 4).

To investigate the relative importance of addressing the sequential emplacement of waste packages in the MSTHM, two different cases were considered. In the 'sequential-emplacement' case, waste packages are sequentially emplaced in the five repository panels. In the SMT submodel, this is implemented on a 20-m by 20-m basis along each of the emplacement drifts, with each 20-m interval having its own unique time of emplacement (i.e., starting time for heating). In the drift-scale submodels (including the LDTH, SDT, and DDT submodels), the starting time of heating is equal to the starting time in the corresponding SMT-submodel grid block. In the 'simultaneous-emplacement' case, waste packages are simultaneously emplaced in all MSTHM submodels at the midpoint (~26 yr) of the 52-yr emplacement period.

A process for representing the influence of repository-scale K_{th} heterogeneity in the host-rock units was developed for the MSTHM. A total of 50 geostatistically varying realizations at a length scale of K_{th} heterogeneity of 50 m were provided by Ramsey [9]. It should be noted that the grid blocks representing the heated portions of the emplacement drifts in the SMT have horizontal dimensions of 20 m (along the drift axis) by 81 m (perpendicular to the drift axis). Because the heterogeneity length scale is roughly equal to the horizontal dimensions of the heated grid blocks for the SMT, and because the length scale is roughly equal to the horizontal dimensions of the LDTH/SDT/DDT submodel, K_{th} heterogeneity is incorporated in a "layer-cake" fashion for all submodels. Repository-scale K_{th} heterogeneity is addressed within each of the four primary host-rock units, including the Tptpul, Tptpmn, Tptpll, and Tptpln units, where Tptp stands for Topopah Spring, 'l' stands for lithophysal, n stands for nonlithophysal, and 'u', 'm', and 'l' stand for upper, middle, and lower, respectively. The model host-rock units are tsw33 (Tptpul), tsw34 (Tptpmn), tsw35 (Tptpll), tsw36 (Tptpln), tsw37 (Tptpln), and tsw38 (Tptpln). At the P5R11C3 location (see Figure 4), the

MSTHM was used to analyze a set of 50 heterogeneous-K_{th} realizations.

Prior to conducting sensitivity analyses for this MSTHM effort it was necessary to test three different approaches to representing repository-scale K_{th} heterogeneity. These three approaches, which are differentiated on the basis of number of submodel types in which K_{th} heterogeneity is represented, are as follows:

1. A "comprehensive" approach incorporates the repository-scale K_{th} heterogeneity in all four of the MSTHM submodels (LDTH, SMT, SDT, and DDT).

2. The "LDTH-only" approach incorporates the repository-scale K_{th} heterogeneity in only LDTH submodels.

3. An "LDTH-DDT-only" approach incorporates repository-scale K_{th} heterogeneity in the LDTH and DDT submodels.

A comparison of waste-package and drift-wall temperatures for the three approaches to incorporating repository-scale K_{th} heterogeneity is given in Figure 5. Waste-package temperature (shown in red) and drift-wall temperature (shown in blue) for the P5R11C3 location is compared for three different approaches to representing repository-scale K_{th} heterogeneity. The influence of repository-scale K_{th} heterogeneity in the DDT submodels is extremely small. Including K_{th} heterogeneity at the 50-m scale in a layer-cake fashion in the DDT submodels has little effect on temperatures. The primary purpose of the DDT submodels is to calculate waste-package-to-waste-package deviations in temperature along the drift and the temperature difference between the waste package and drip shield. Neither of these quantities is influenced by K_{th} heterogeneity at the 50-m scale.

Representing K_{th} heterogeneity in the SMT submodel does not affect peak temperatures (Figure 5); however, it has a small but noticeable effect on temperatures during the 300 to 2000 yr timeframe. The primary purpose of the SMT submodels is to determine the rate at which the 'edge-cooling' effect influences local temperatures. At the P5R11C3 location, the edge-cooling effect requires several hundred years to be manifested. Consequently, the small influence of repository-scale K_{th} heterogeneity in the SMT submodels is not felt until about 300 yr. Because the evolution of the edge-cooling effect is weakly affected by repository-scale K_{th} heterogeneity, it is not necessary to include K_{th} heterogeneity in the SMT submodels. In summary, these observations indicate that it is only necessary to represent repository-scale K_{th} heterogeneity in the LDTH submodels.

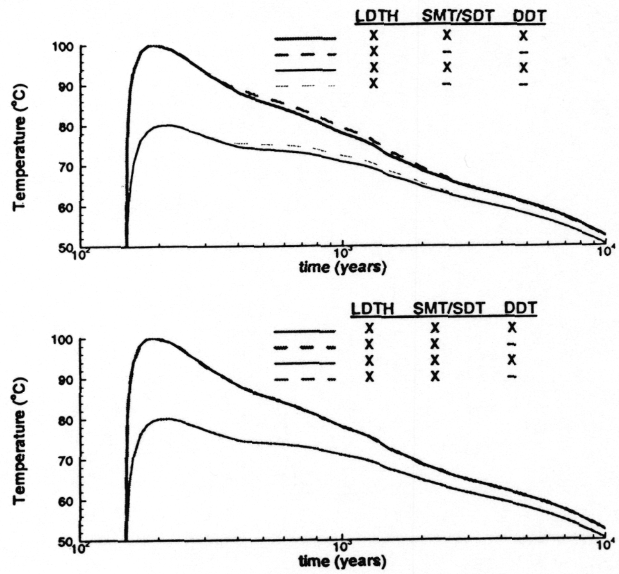

Figure 5. Waste-package temperatures (shown in red) and drift-wall temperatures (shown in blue) for the P5R11C3 location are compared for three different approaches to representing repository-scale K_{th} heterogeneity.

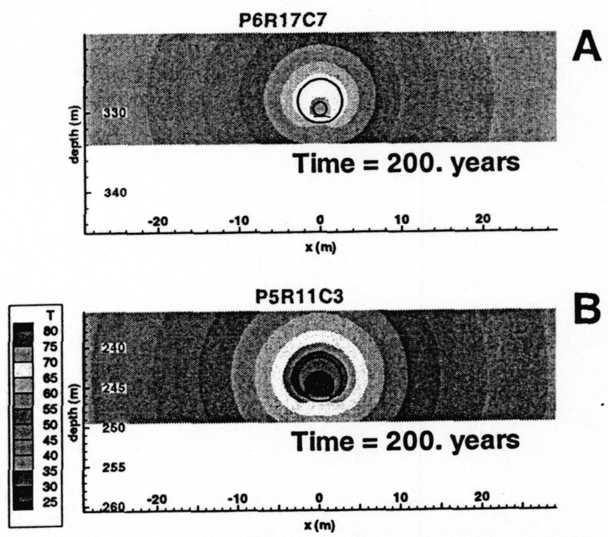

Figure 6. A vertical cross section of temperatures at 200 yr is shown (plot A) for the P6R17C7 location, which is near the repository edge and where waste packages are emplaced towards the end of the emplacement period. Temperatures are also shown (plot B) at 200 yr for the P5R11C3 location, which is near the center of the repository and where waste packages are emplaced towards the end of the emplacement period. Temperatures are "line-averaged" for a sequence of 10 waste packages.

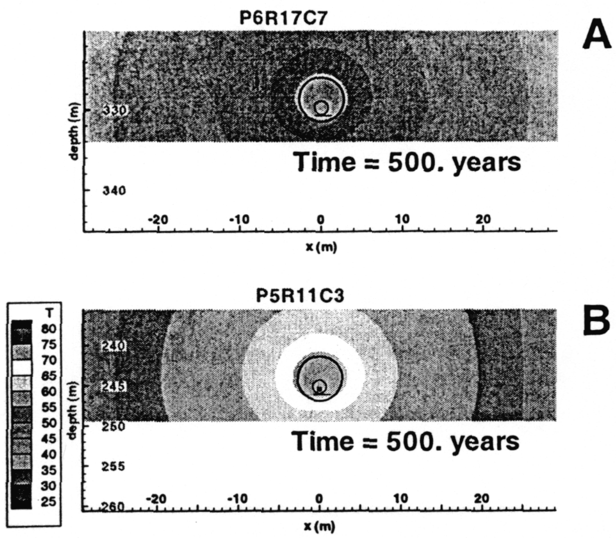

Figure 7. A vertical cross section of temperatures at 500 yr is shown (plot A) for the P6R17C7 location, which is near the repository edge and where waste packages are emplaced towards the end of the emplacement period. Temperatures are also shown (plot B) at 500 yr for the P5R11C3 location, which is near the center of the repository and where waste packages are emplaced towards the end of the emplacement period. Temperatures are "line-averaged" for a sequence of 10 waste packages.

RESULTS

Recent improvements to the MSTHM are applied to the long-duration preclosure ventilation case. Waste packages are spaced apart by an average of 2 m to yield a line-averaged thermal load of 1.15 kW/m of emplacement drift and are sequentially emplaced throughout the repository during a 52-yr period. Forced ventilation of the drifts occurs for 98 to 150 yr, with 98 yr applying to the last emplaced waste package and 150 yr applying to the first emplaced waste package. The same generic heat-generation curves for each of the respective waste-package types are used throughout the repository, with the onset of heating corresponding to the local time of emplacement. For example, the first emplaced waste packages have curves shifted by 0 yr, while the last emplaced waste packages have curves that are shifted by 52 yr.

The ability of the MSTHM to represent TH conditions both within the emplacement drift and in the host rock is demonstrated in Figure 6 and Figure 7, which show the line-averaged temperatures for a location close to the repository edge (P6R17C7) and one close to the repository center (P5R11C3). At these locations, waste packages are emplaced towards the end of the emplacement period. A comparison of Figure 6 and Figure 7 clearly shows the influence of the edge-cooling effect. The edge location cools down much more quickly than the center location. Also note that for the center location the radial extent of the zone of temperature rise is still expanding at 500 yr, while for the edge location it is not.

Of particular importance in this modeling study is the ability to represent a complex repository layout, consisting of multiple panels (Figure 1), as well as the ability to represent sequential emplacement of waste packages. Prior to this study, all MSTHM analyses assumed a repository layout with a single contiguous panel with all waste packages simultaneously emplaced [1,2,3,4]. To evaluate the relative importance of representing sequential emplacement, a recent MSTHM study compared the results of a case that assumed simultaneous waste-package emplacement with those that represented sequential waste package emplacement. Figure 8 compares waste-package temperatures for the simultaneous-emplacement and sequential-emplacement cases for a location where waste packages are emplaced during the early portion of the emplacement period. Figure 9 makes the same comparison for a location where waste packages are emplaced during the latter portion of the emplacement period. The assumption of simultaneous emplacement results in higher peak temperatures than the sequential-emplacement case for locations that are emplaced early (Figure 8), while this assumption results in slightly lower peak temperatures for locations that are emplaced during the latter portion of the emplacement period (Figure 9).

For the sequential-emplacement case, greater-than-average heat-output waste packages generally result in above-boiling temperatures, particularly for waste packages emplaced towards the end of the emplacement period. Less-than-average heat-output waste packages (e.g., HLW waste packages) generally never result in above-boiling temperatures. It is important to note that these observations apply to a case with a prolonged preclosure ventilation period, ranging from 98 to 150 yr.

The influence of repository-scale K_{th} heterogeneity was evaluated using a geostatistical variation about average K_{th} values. A total of 50 realizations were considered, varying K_{th} at a heterogeneity length scale of 50 m. The set of 50 realizations is run incorporating K_{th} heterogeneity only in the LDTH submodels. Variation in waste-package temperature for the 50 realizations at location P5R11C3 is illustrated in Figure 10 for the hottest package, PWR1-2, and in Figure 11 for the coolest package, DHLW-L2. The maximum range in waste-package temperatures is about 11.5°C at a time of 180 yr for these 50 realizations. This deviation is half the maximum spread between hottest and coolest packages, which is about 25°C at 180 yr.

CONCLUSIONS

The following conclusions can be drawn from the recent MSTHM modeling effort:

1. Superposition of SMT-submodel temperatures can accommodate complex emplacement drift/panel layouts, including multiple non-parallel emplacement planes.

2. Waste-package sequencing and location within the repository significantly influence host-rock and waste-package temperatures.

3. SMT and DDT submodels do not need to incorporate thermal-conductivity heterogeneity for the heterogeneity length scales at least as large as that considered in this study (50 m).

4. Sequential waste-package emplacement is an important modeling consideration because MSTHM results are influenced by the duration of the ventilation period. Note that this conclusion particularly holds for situations with a prolonged period of emplacement (e.g., the 52-yr emplacement period considered here). For shorter emplacement durations (e.g., 25 yr), the differences in thermohydrologic conditions between the earliest and latest emplaced waste packages will be less.

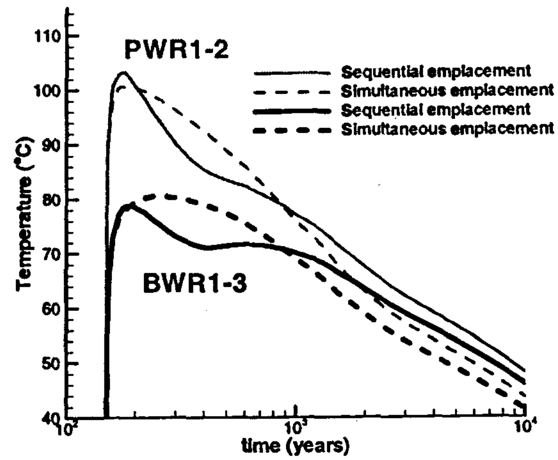

Figure 9. Waste-package temperature histories are given for a PWR and a BWR CSNF waste package at a location emplaced during the latter portion of the emplacement period (P5R11C3). The case that assumes simultaneous emplacement of waste results in slightly lower peak temperatures than those predicted for the case accounting for sequential emplacement.

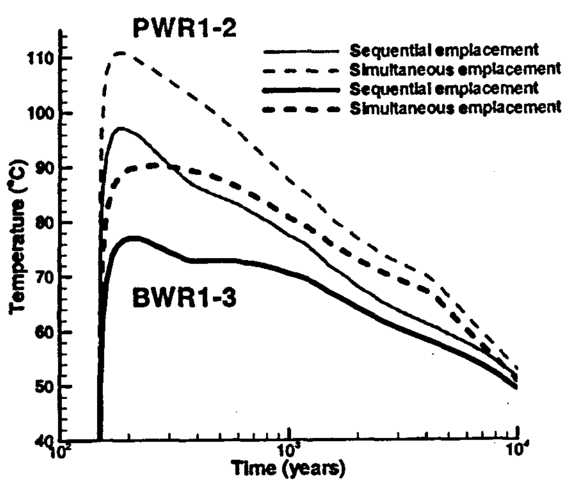

Figure 8. Waste-package temperature histories are given for a PWR and a BWR CSNF waste package at a location emplaced during the early portion of the emplacement period (P4R8C5). The case that assumes simultaneous emplacement of waste results in higher peak temperatures than a case accounting for sequential emplacement.

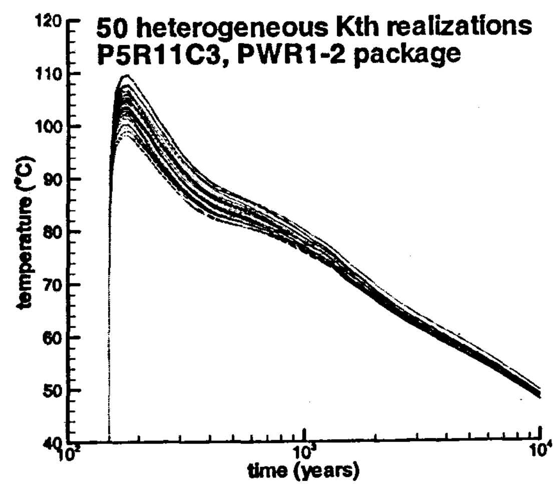

Figure 10. For waste-package temperature at 180 yr, the 50 repository-scale heterogeneous K_{th} realizations at location P5R11C3 result in a spread of 11.4°C for the PWR1-2 CSNF waste package. Note that this waste package has the highest heat output of those considered in these analyses.

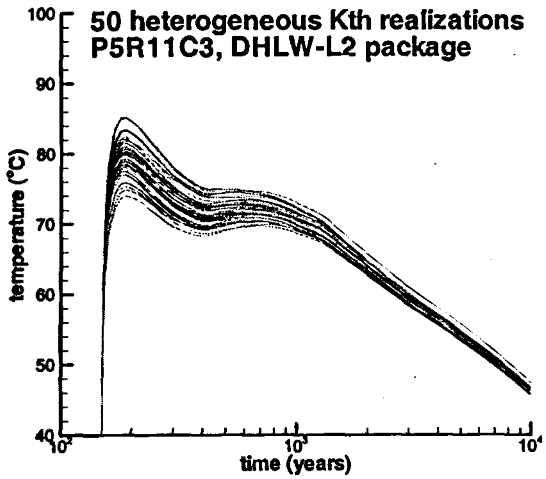

Figure 11. For waste-package temperature at 180 yr, the 50 repository-scale heterogeneous K_{th} realizations at location P5R11C3 result in a spread of 11.5°C for the DHLW-L2 waste package. Note that this waste package has the lowest heat output of those considered in these analyses.

ACKNOWLEDGEMENTS

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